Stretch Efficiency for Combustion Engines: Exploiting New Combustion Regimes

Project ID: ACS015

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Project Overview

BARRIERS (MYPP, SECTION 2.4, CHALLENGES AND BARRIERS C.)

Lack of fundamental knowledge of advanced engine combustion regimes.

…inadequate understanding of the fundamentals of thermodynamic combustion losses

…inadequate capability to accurately simulate these processes

BUDGET

- FY15: $300k
- FY16: $300k
- FY17: $275k

(~ 0.5 FTE + materials)

PROJECT TIMELINE

- ***Project was started in FY17 through the Combustion Lab Call (FY17-FY20)***
- ***Builds on prior Stretch Efficiency research program at ORNL***
  - ***Focus on thermochemical recuperation in 2011***

INDUSTRIAL PARTNERSHIPS AND COLLABORATION

- ***Ford – Providing technical input***
- ***AEC working group led by SNL***
  - ***Mechanism for industry feedback***
- ***Aramco Services – Technical collaboration***
- ***ANSYS (formerly Reaction design) – CFD model development***
- ***Umicore – Catalyst coatings***

Universities

- ***University of Michigan - Galen Fisher***
- ***University of Michigan – Yan Chang***

National Labs

- ***Sandia National Laboratories – Isaac Ekoto***

Relevance: Decreased Petroleum Consumption through Higher Engine Efficiency

Project Overview
Relevance
Milestones
Approach
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Summary

Overall Project Goal

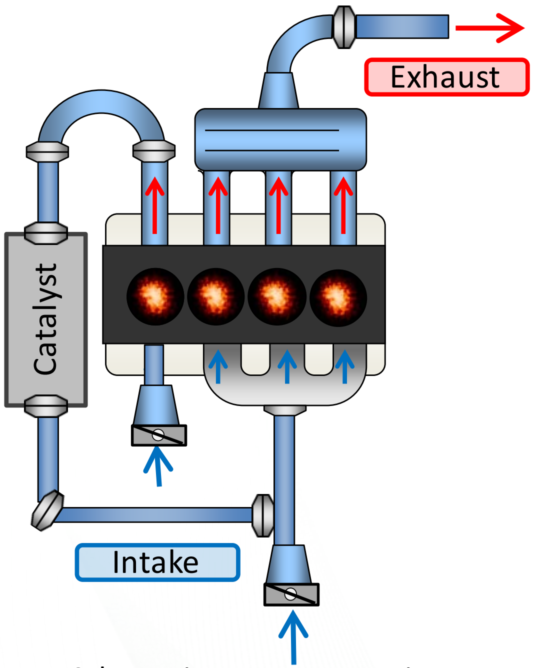
- Increase IC engine efficiency with an approach centered on thermodynamic of engine processes and minimizing losses

Constraints

- Stoichiometric operation to maintain compatibility 3-way catalyst
- Compatible with regular-grade gasoline

Project History

- Thermochemical recuperation through reforming has been pursued for several years
  - Results indicate that in-cylinder reforming is not as promising as originally thought
  - Bench flow reactor results indicate promise for catalytic reforming



Note: Schematic represents engine flow paths and is not intended to represent instrumentation or controls

- This presentation contains the first results from on-engine catalytic EGR loop reforming

This Project has One Tracked Milestone for FY17

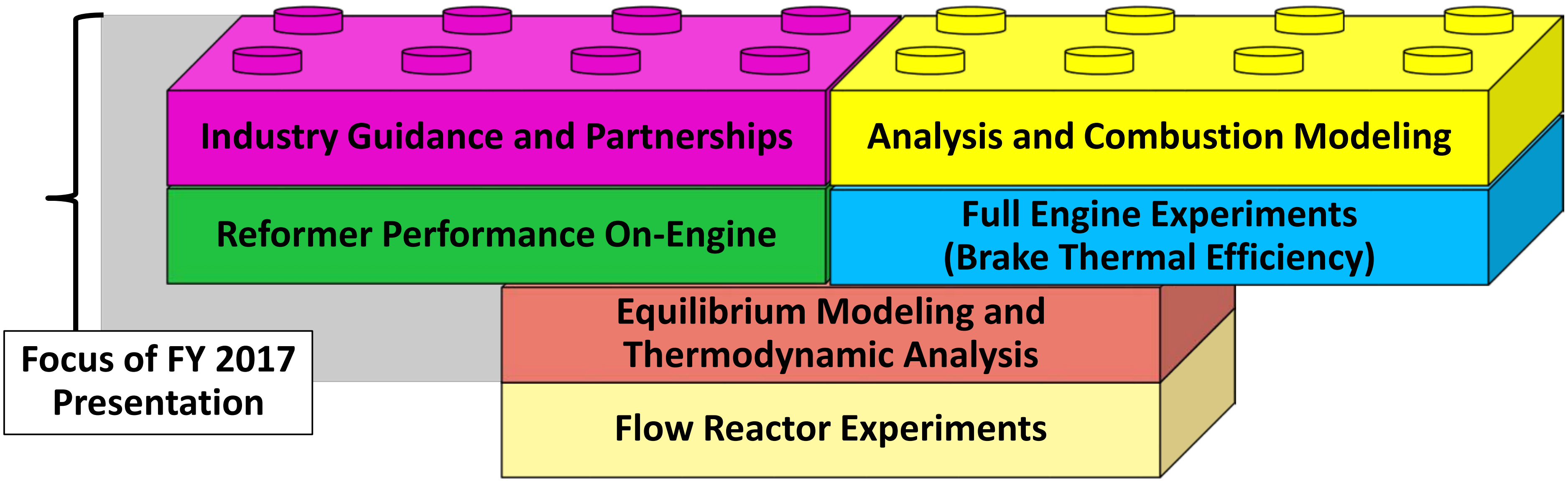
Third Quarter, FY2017

Complete a map of the performance of the catalytic reforming strategy on the engine as a function of inlet conditions.

Status: Complete

Data-Based Decision Presented at 2016 AMR to Focus on Catalytic Reforming over In-cylinder Reforming

Approach (1/3)



Flow Reactor Experiments from Prior Years Guiding FY 2017 Approach

- Steam reforming alone is not promising (reactions enthalpy-limited, poor sulfur tolerance)
- Partial oxidation reforming can produce high reformate yield and achieve thermochemical recuperation
  - Energy balance is a strong function of equivalence ratio, operate $3 < \Phi < 10$
  - Improved tolerance to sulfur and low catalyst inlet temperature conditions

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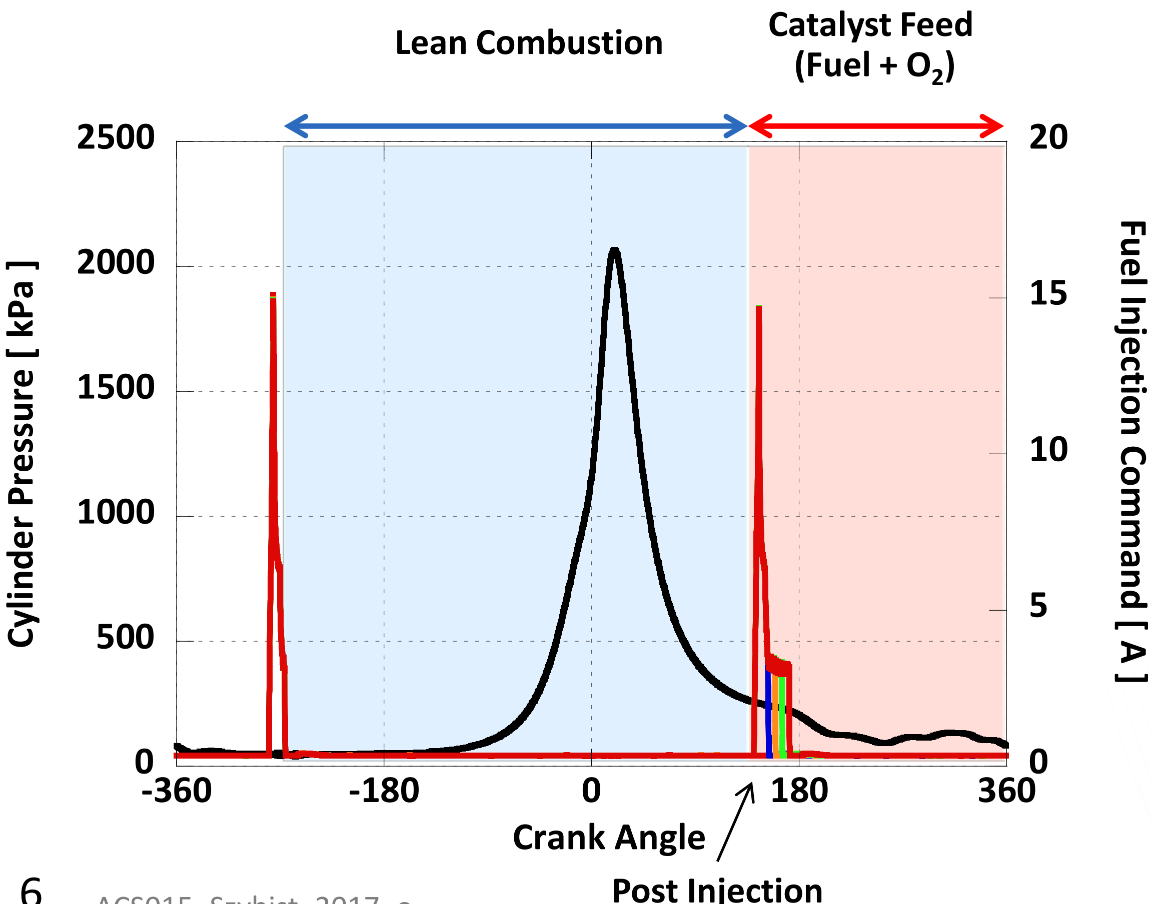
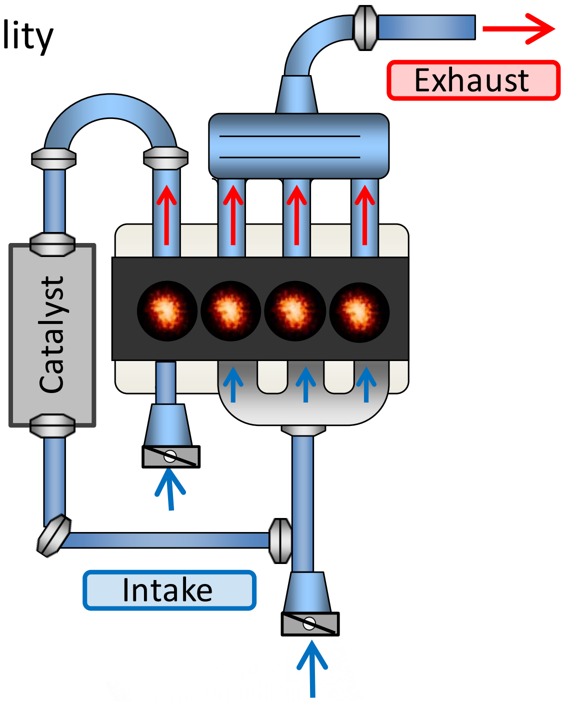
Implementation of the EGR Loop Reforming on an Engine: Providing Oxygen to the Reforming Catalyst will Require Lean Operation

Approach (2/3)

- Lean combustion by one cylinder to feed oxygen to reforming catalyst
  - Allows stoichiometric exhaust for 3-way exhaust TWC compatibility
  - Allows lean cylinder to be at a higher MAP, match load
- Fuel provided to catalyst through post injection event



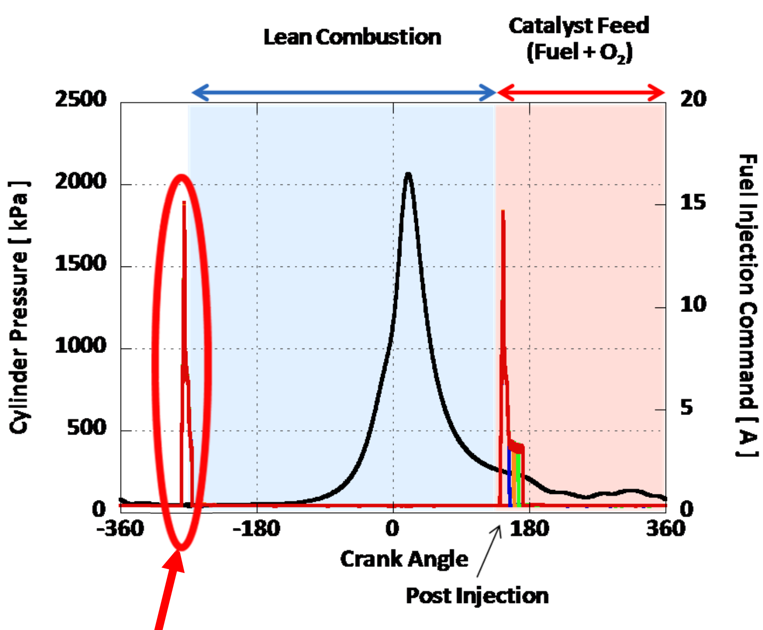


Catalyst Details

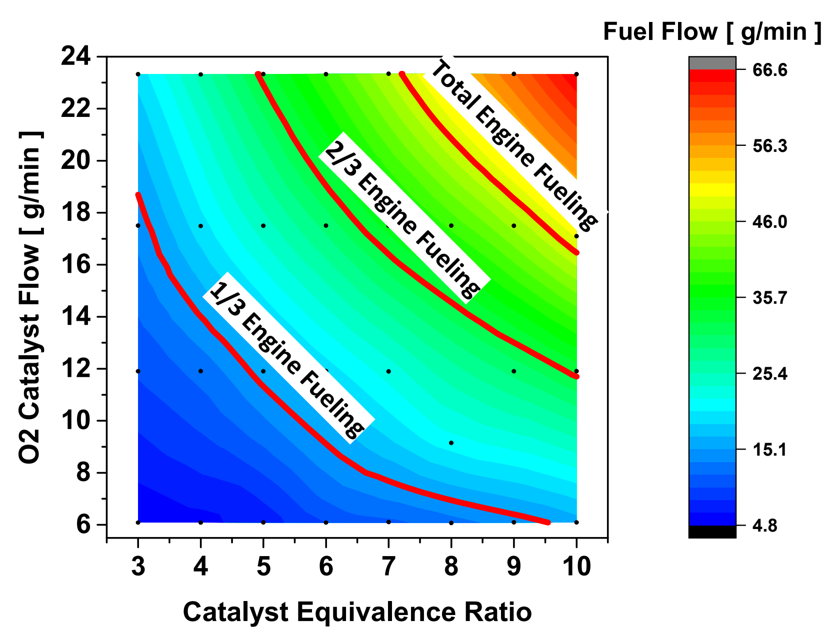
- 2 wt% Rh, alumina washcoat
- 2 x 0.75 L cordierite bricks
- 400 cpsi
- Catalyst originally developed by Delphi

Results will be Presented on a Basis of Oxygen Flow Rate and Equivalence Ratio Into the Catalyst

- Experiments use constant engine speed (2000 rpm) and constant main injection duration (16.0 mg/injection) with iso-octane (comparison to gasoline at end of presentation)
  - This targets a 2000 rpm, 4 bar BMEP (~20% load) operating condition (ACEC part load condition)
- Results are presented using contour plots
  - Y-Axis: Excess combustion air that goes to catalyst (presented as $\dot{m}_{O2}$)
  - X-Axis: Equivalence ratio at catalyst (dictated by post injection duration)
- Investigated post-injection fueling spans from < 10% to > 100% of the fuel for cylinders 1-3



Main Injection Constant



Energetic Differences Between Steam and Partial Oxidation Reforming. Our Approach Uses a Combination.

- Energy balance highly fuel-dependent (C/H)
- POx consumes fuel energy

$$C_8H_{18} + 4*(O_2 + 3.76\ N_2) \rightarrow 8\ CO + 9\ H_2 + 15.04\ N_2$$

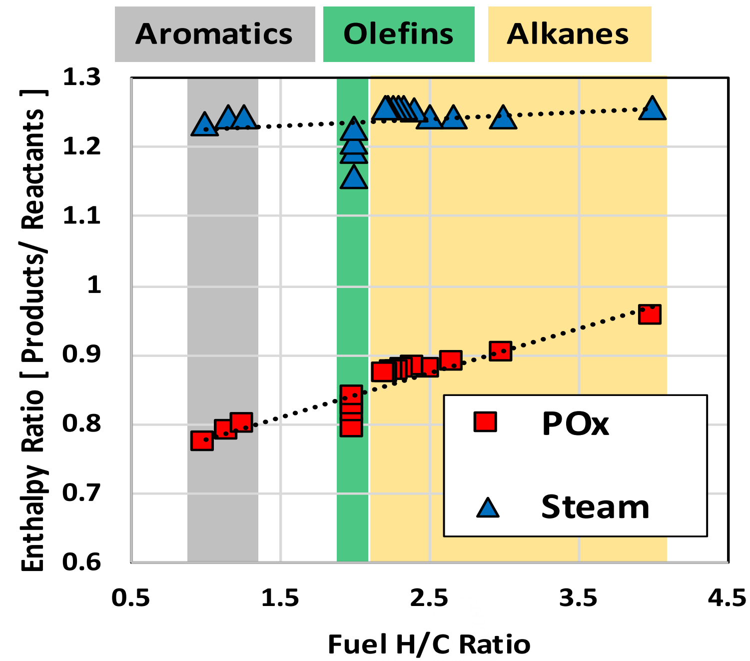
POx reforming with iso-octane, C:O = 1

- Steam reforming is the route to thermochemical recuperation

$$C_8H_{18} + 8\ H_2O \rightarrow 8\ CO + 17\ H_2$$

Steam reforming with iso-octane

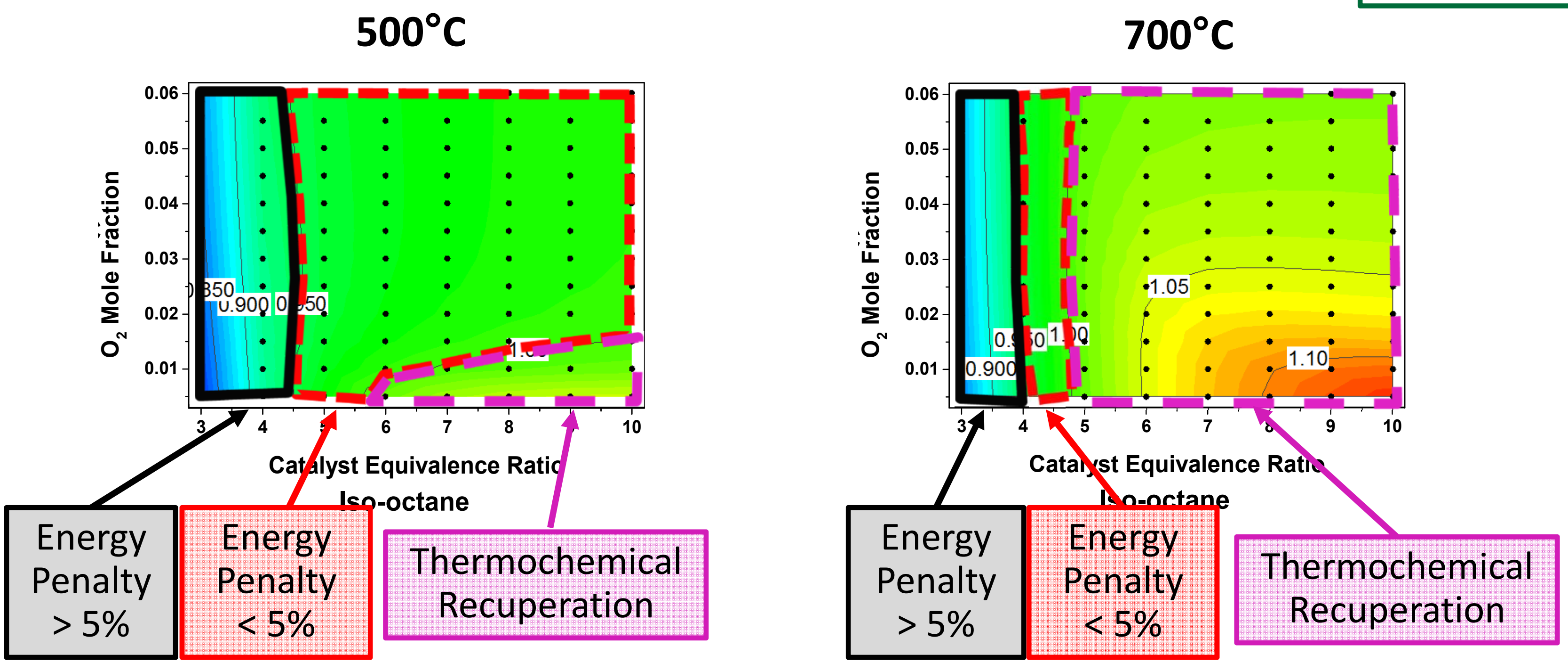
- Optimal reforming conditions may differ based on desired outcome – highly dependent on engine response
  - Highest H_2 yield
  - Most favorable reforming energetics
  - **Best overall engine efficiency**



Equilibrium Modeling and Thermodynamic Analysis

Equilibrium Modeling Shows that Initial Temperature Matters to Energy Balance; Thermodynamics are Enthalpy Limited

Accomplishments (2/12)

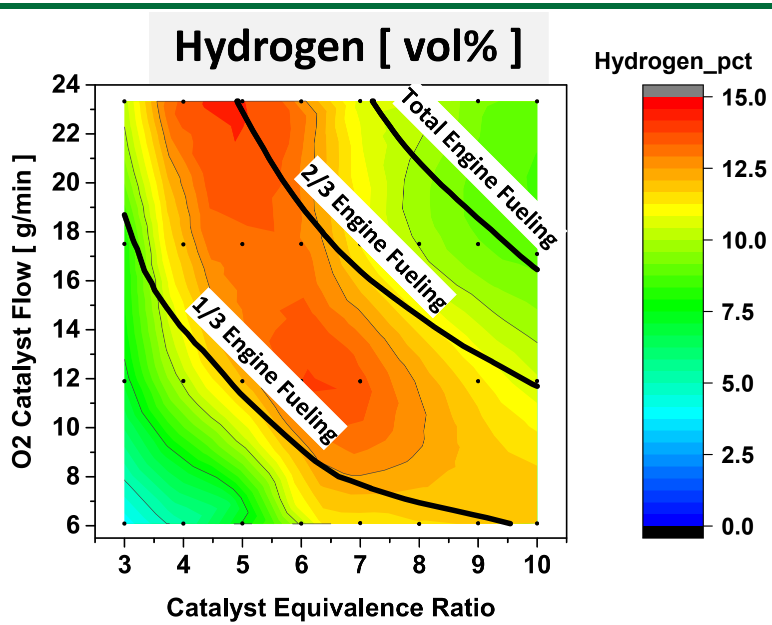


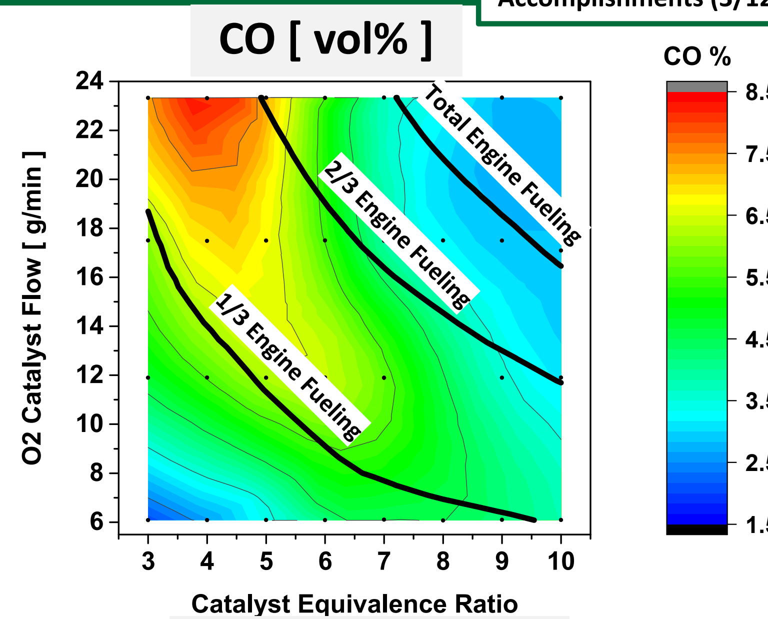
- Chemical equilibrium calculations performed using Chemkin, LLNL detailed gasoline surrogate mechanism
- Operating conditions matched to experimental map
- Enthalpy of formation at standard conditions for chemical constituents

Equilibrium Modeling and Thermodynamic Analysis

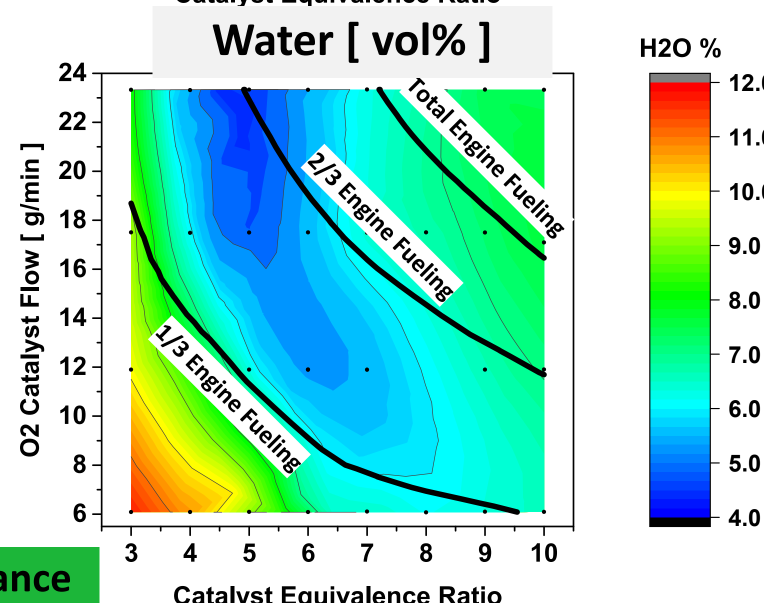
Quasi Steady-State Reforming Products Highly Dependent on Equivalence Ratio and O_2 Flowrate into Catalyst

Accomplishments (3/12)



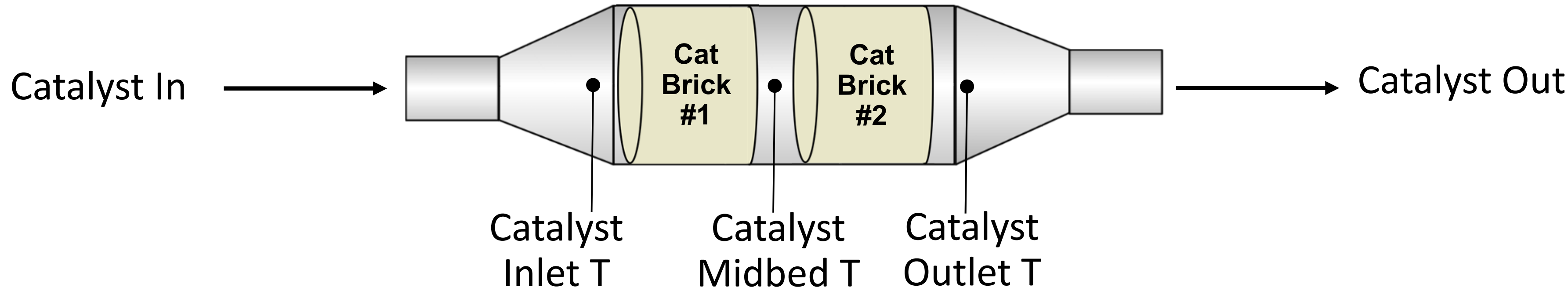


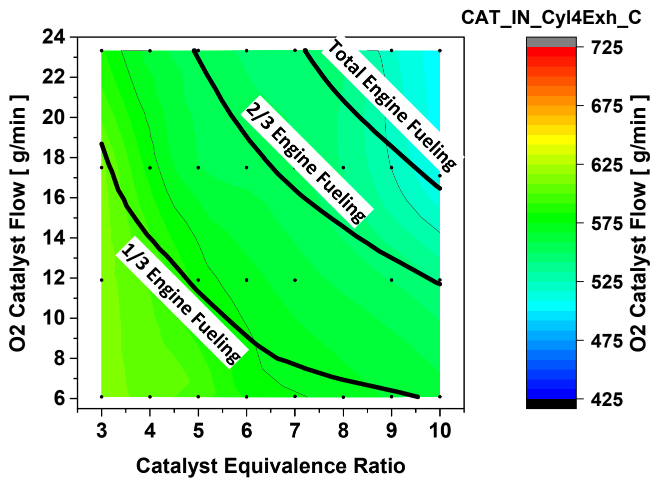
- Regions of maximum H_2 and CO correspond with region of minimum H_2O
  - Corresponds to ~40-60% of fuel for remaining cylinders going through catalyst, with catalyst Φ = 4-7
- Low water concentration is evidence of steam reforming activity
  - Water gas shift favored at higher Φ



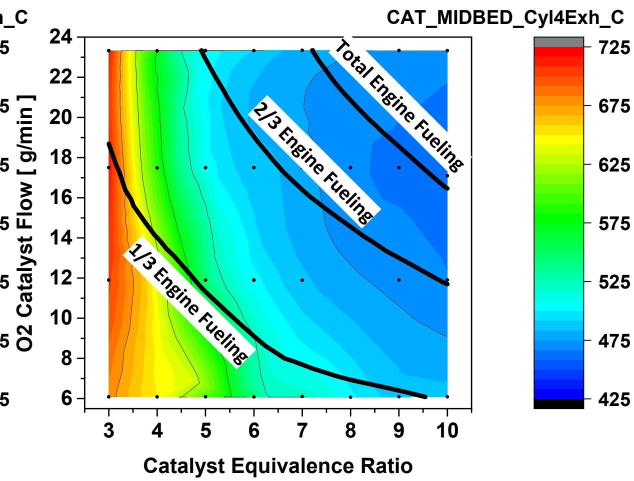
Reformer Performance on-Engine

Thermal Analysis of the Catalyst Operating on Engine: Exothermic and Endothermic Reactions Observed, Dependent on Φ

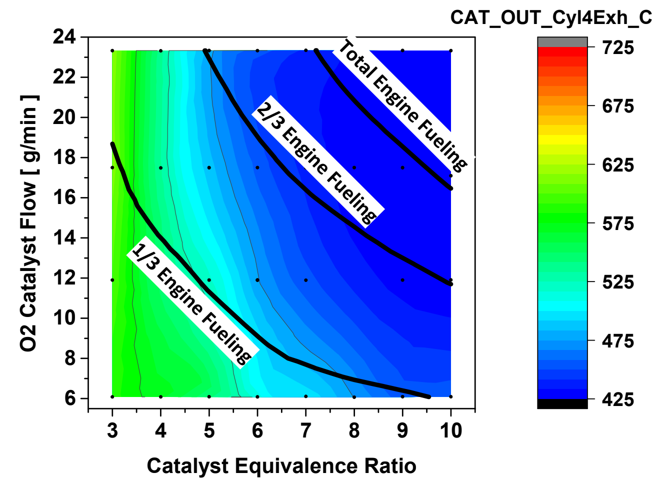




- Only small variations in catalyst inlet temperature
- Variations attributed to dilution and combustion phasing effects



- Midbed catalyst temp shows evidence of both endothermic and exothermic reactions
- Energetics are dependent on equivalence ratio



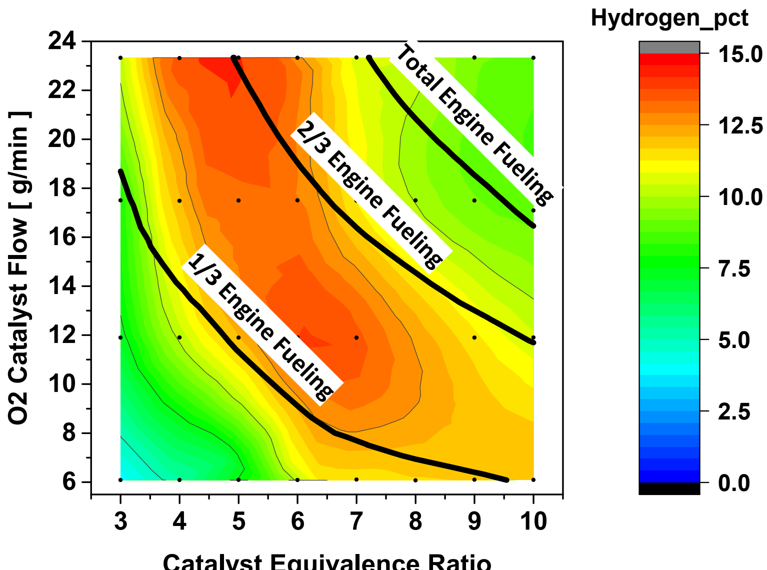
- Catalyst out temperature is significantly lower than the inlet temperature
- Higher equivalence ratios all approach the same outlet T

Reformer Performance on-Engine

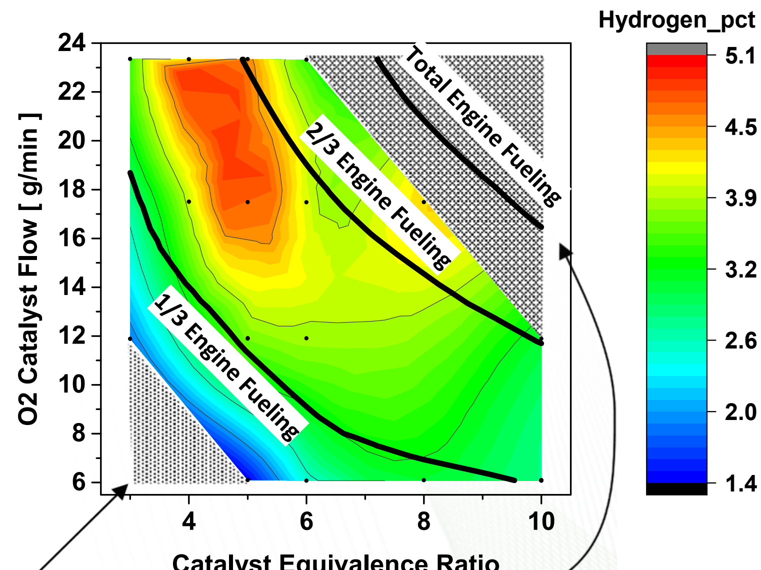
Reformer-Out H_2 Concentration up to 15% Yields Intake Manifold H_2 Concentration up to 5%

- Operable engine space is smaller than the mapped catalyst space
  - Data collected only where COV of IMEPg < 5% in all cylinders
- The way that the experiments were run, mass flow rate over the catalyst varied
  - Increasing the O_2 catalyst flow increases mass flow rate
  - Increasing catalyst equivalence ratio increases mass flow rate

Catalyst Mapping
Concentrations at Catalyst Outlet



Multi-Cylinder Engine Operation
Concentrations in Intake Manifold



Engine not operable

Full Engine Experiments (Brake Thermal Efficiency)

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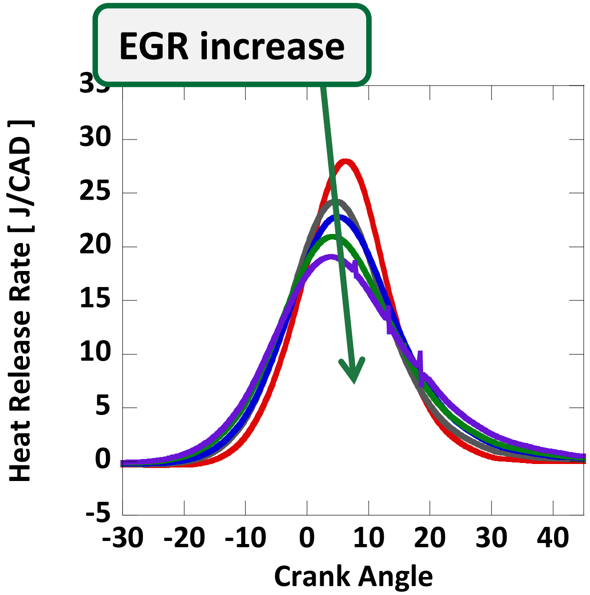
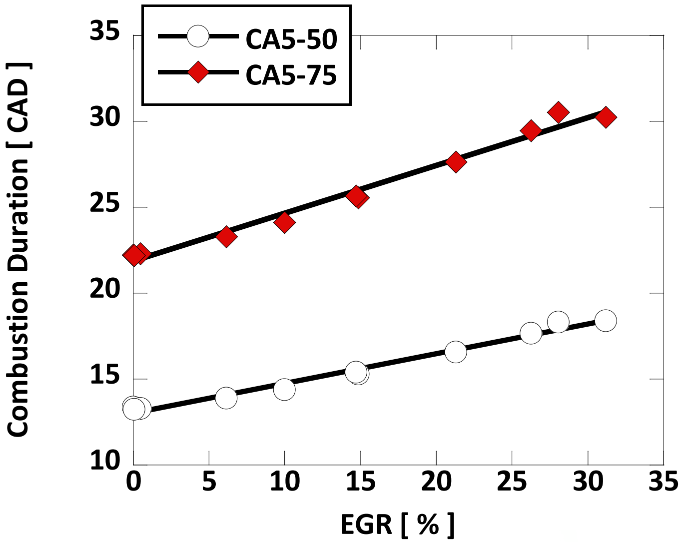
With Conventional EGR in SI Engines, Combustion Duration Elongates and the Peak Heat Release Rate Decreases





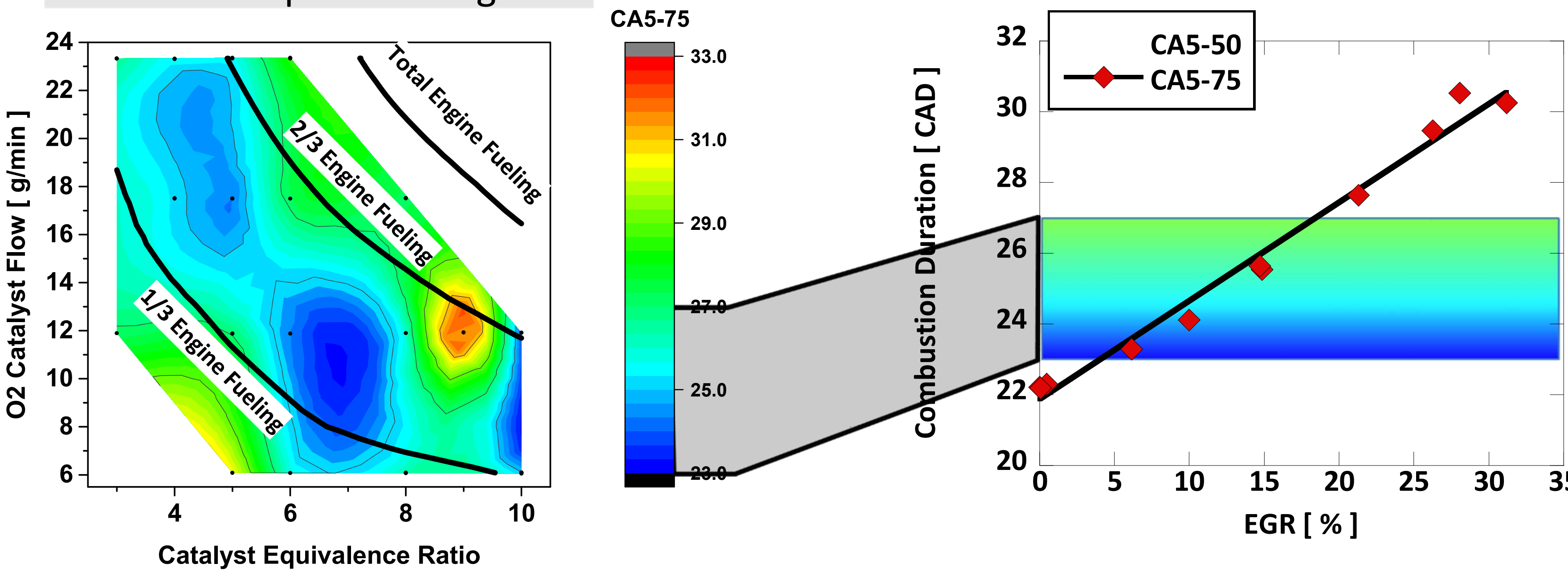
- Peak heat release rate drops > 30%
- EGR elongates every portion of the combustion duration (flame kernel development, turbulent combustion duration, and combustion burn-out)
- Combustion elongation adversely effects efficiency
  - Competes against higher polytrophic coefficient, reduced heat transfer
  - Longer initial flame kernel development leads to higher combustion instability

Full Engine Experiments (Brake Thermal Efficiency)

Combustion Duration Achieved with Catalytic EGR Reforming is Comparable to about 10-20% Conventional EGR

CA5-75 Combustion Duration: EGR Loop Reforming

CA5-75 Combustion Duration: Conventional EGR



- Combustion duration changes due to reforming conditions (oxygen flow and catalyst equivalence ratio)
- CA5-75 combustion duration of 23.5 CA is comparable to ~10% conventional EGR
- Amount of EGR is difficult to quantify, because, what is EGR?

Full Engine Experiments (Brake Thermal Efficiency)

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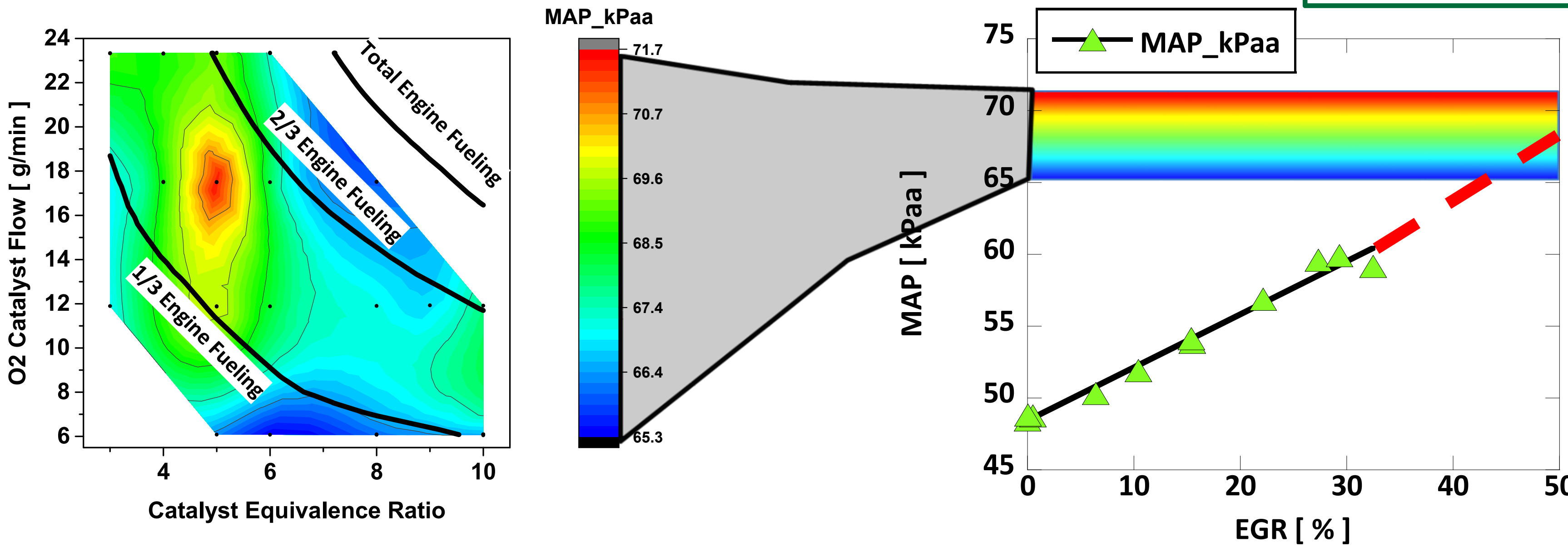
Functional EGR Level from a Pumping Perspective Approaches 50% with Catalytic Reforming Strategy

Accomplishments (8/12)



- With conventional EGR, linear trend exists between intake manifold pressure and EGR
- Still working on how to quantify EGR for catalytic reforming strategy
  - EGR stream contains significant portion of the fuel energy for the combustion event. It is not "exhaust gas"
- From a pumping perspective (PMEP), MAP is the important factor
  - From extrapolation of MAP, catalytic reforming is equivalent to 40-50% EGR
  - This makes sense! Configuration leads to 33% EGR if all cylinders are operating the same. Combustion is lean. Volume increase over catalyst for reforming process.

Full Engine Experiments (Brake Thermal Efficiency)

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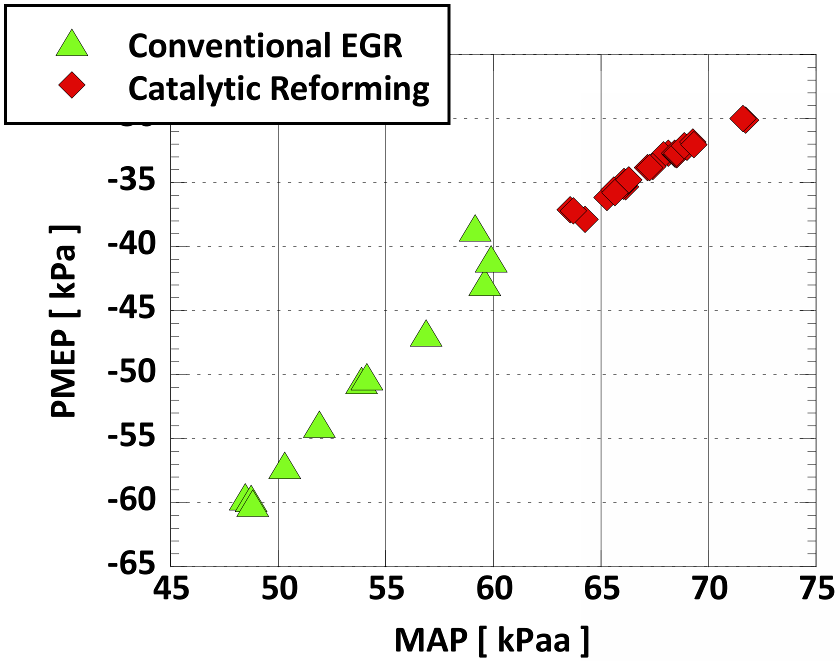
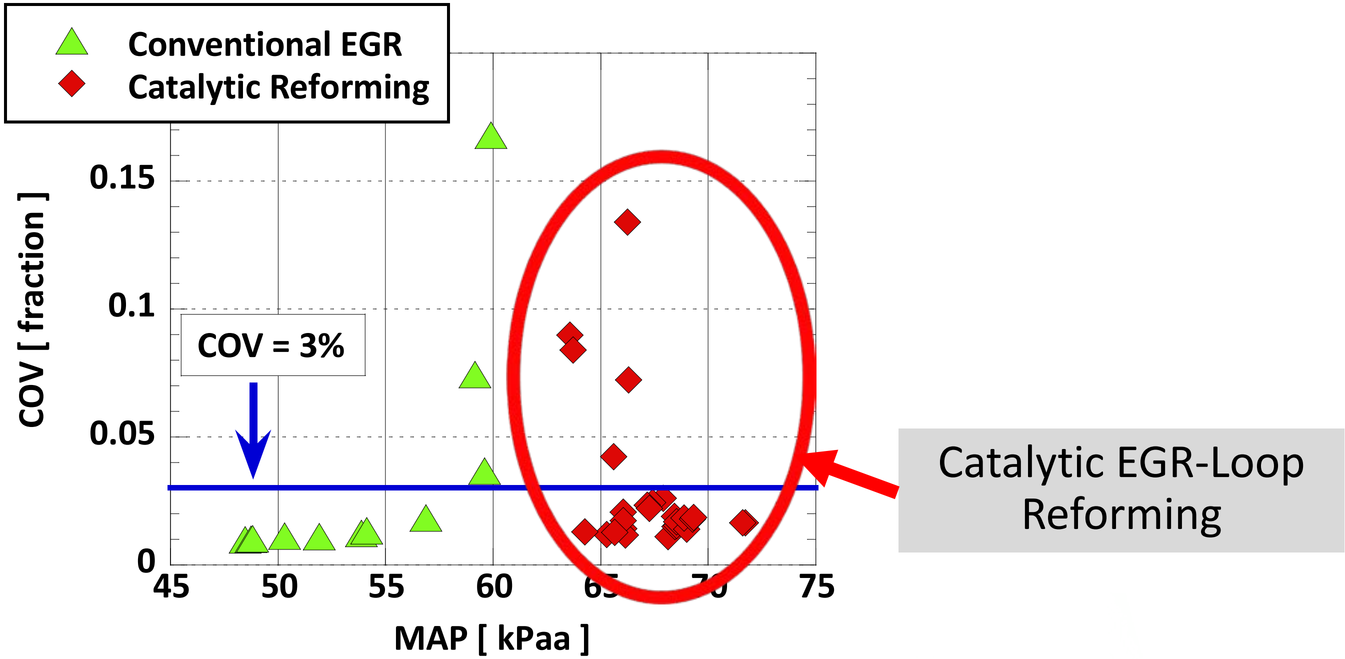
Plot of PMEP vs. MAP Confirms the Volumetric EGR Trend



Full Engine Experiments (Brake Thermal Efficiency)

Catalytic Reforming Allows EGR and MAP to be Increased Without Increase in Combustion Instability

Accomplishments (10/12)

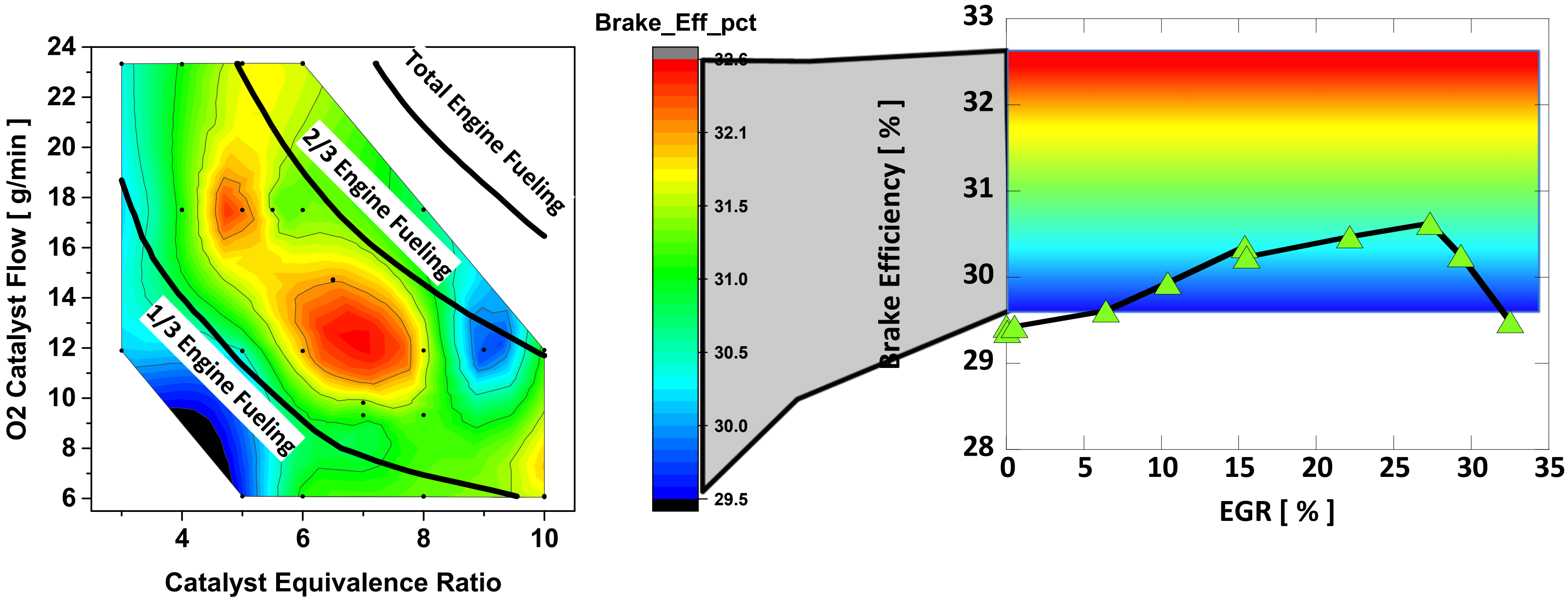


- Conventional EGR "hits the stability wall" as EGR increases
  - Non-linear increase in instability as EGR and MAP increase with both gasoline and iso-octane
- Catalytic EGR enables significant increase in MAP with comparable stability to 0-10% EGR

Full Engine Experiments (Brake Thermal Efficiency)

Brake Efficiency Increased by as much as 3 Efficiency Points over Baseline Operating Condition without EGR

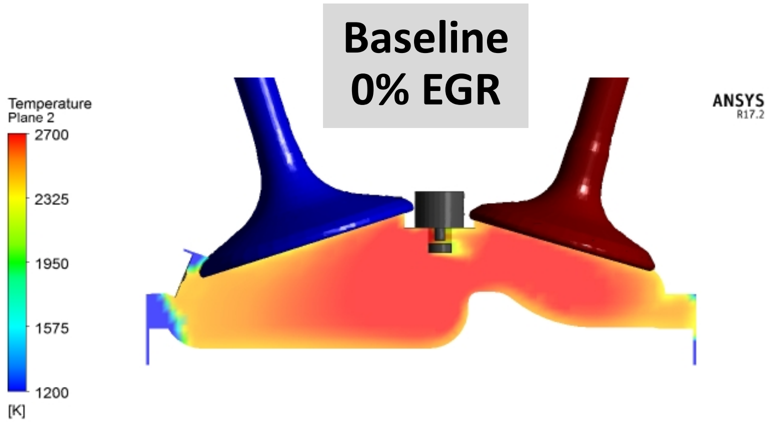
Accomplishments (11/12)

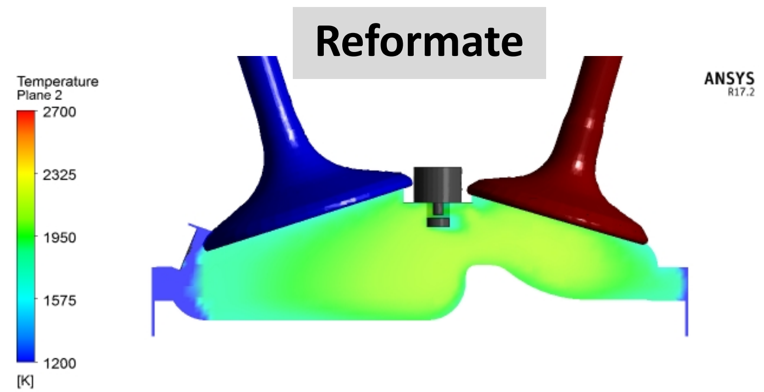


- This efficiency benefit equates to ~10% fuel consumption reduction at a part-load condition
- This "base" efficiency improvement is substantial, but may just be the start
  - Current study used constant fueling to cylinder feeding reforming catalyst, which resulted in lack of cylinder balance. Possible efficiency benefits to balancing cylinders
  - Known knock benefit with EGR, thus further efficiency benefits may be possible with higher compression ratio
  - Many more hardware configuration possibilities…

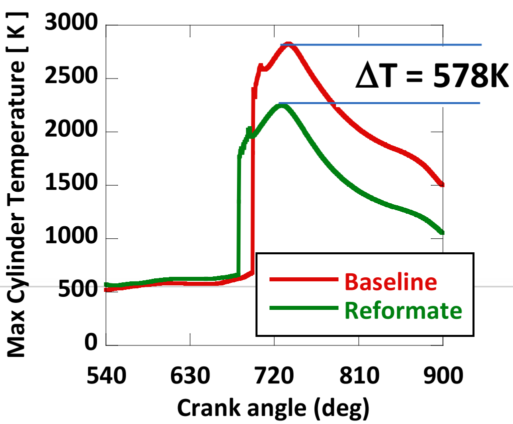
Full Engine Experiments (Brake Thermal Efficiency)

Initial Modeling Reveals Large Reductions Temperature and Heat Transfer, Increases in Indicated Efficiency

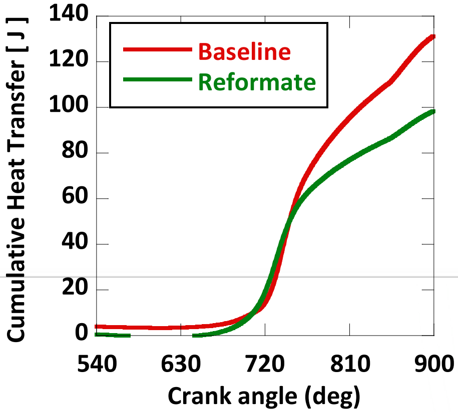




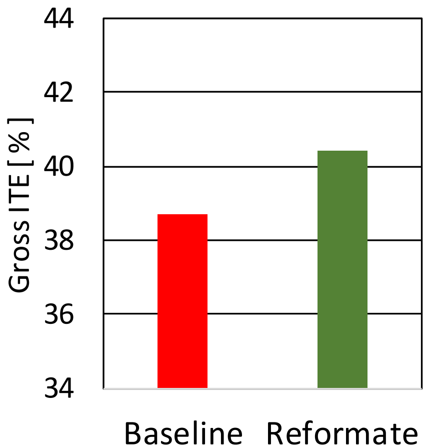
Simulation: 2000 RPM, 655-665 J Chemical Heat Release



With large decrease in cylinder T, approaching λ=1 LTC with a flame!!!



Heat transfer decreased by 25%. Substantial increase in gamma (combined composition and T).



Indicated efficiency increase of 2 percentage points (without pumping benefits)

Analysis and Combustion Modeling

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Six Reviewers Evaluated the Predecessor to this Project in 2015 (ACE015) Overall Positive Comment with Room for Improvement

Several reviewers commented on the need to bring an OEM partner on-board

Ford is now a collaborator and is interested in keeping track of this work. Progress is presented to Ford in a one-on-one setting, and they offer input to where they see challenges to implementation. Input from Ford was incorporated into the plans for future work.

One reviewer commented that the study needs to be expanded beyond a single speed/load operating point

We agree. There are three planned experimental campaigns, and two of these are focused on load expansion (see future work slide).

Schematics of engine seem to omit details on valves and probes

The schematics were made to highlight the unconventional engine flow patterns in the engine, not as a comprehensive instrumentation schematic.

Several reviewers wanted to see a more direct link to how higher efficiency would be realized: dilution vs. TCR

Ultimately, we hope to have a thermodynamic benefit from both higher dilution and TCR. The experimental results from combustion stability (and pumping benefits) combined with the CFD modeling helped to elucidate the efficiency benefits with increased dilution. The equilibrium modeling of the reforming process was an attempt to capture the thermodynamics of generating the reformate mixture.

One reviewer requested additional information about the catalyst, and requested that we report the effects of different catalyst compositions

Additional information on the catalyst is included in the approach section. This catalyst was originally developed by Delphi for reforming purposes, and this project is building on prior industry expertise. Further catalyst development or testing different catalyst formulations is outside of the project scope.

Collaborations

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- Project direction from 2010 USCAR Colloquium
  http://feerc.ornl.gov/pdfs/Stretch_Report_ORNL-TM2010-265_final.pdf
- OEM Collaboration: one-on-one discussions with Ford
  - Interested in the subject and providing input on implementation barriers
  - Feedback has been incorporated in development of future work plans
- Umicore – Providing pre-production Rh-based catalysts
- ANSYS (formerly Reaction Design) – CFD model development and technical assistance
- University of Michigan: Yan Chang is a UM student working on the project at ORNL for 2016, advised by Stani Bohac and André Boehman
- AEC Working Group bi-annual meetings
  - Mechanism for industry feedback
- University of Michigan: Galen Fisher advising on catalyst formulation and operating conditions through subcontract
- Related funds-in project with Aramco Services Co.
- Sandia National Laboratories: Historical collaboration with Isaac Ekoto (and Dick Steeper). Projects diverged this year, but technical discussions continue.

Industry Guidance and Partnerships

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Barriers and Future Work: Sulfur Tolerance, Expansion of Operating Map

Any proposed future work is subject to change based on funding level

Complete Reporting of Existing Data

- 3 manuscripts nearing journal submission

Barrier: Sulfur can Deactivate Reforming Catalysts

- Real gasoline (10 ppm sulfur) shows decreased performance (backup slides)
- Experimental campaign planned to investigate 0, 10, 20, and 30 ppm sulfur in a common base fuel (doping thiophene into toluene/iso-octane/n-heptane blends)

Barrier: Light Load Stability is Problematic for Highly Dilute Engines

- Engines require stable operation over complete engine operating map
- Experimental campaign planned to characterize light-load catalyst performance, engine stability, and overall system thermodynamics

Barrier: High Efficiency Concepts Must Provide High Power Density

- Power density is critical for SI engines, thus compatibility under boosted conditions is required
- Experimental campaign planned to operate engine under boosted conditions (~12-14 bar BMEP)

Modeling

- Thermodynamic and CFD modeling will continue to be utilized to provide insight

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Relevance

Working to increase efficiency in SI, λ=1 engines through a combination of dilution limit extension and thermochemical recuperation

Approach: Experimental and Modeling Efforts Grounded in Thermodynamics

- Enable catalytic EGR loop reforming on an SI engine
- Flow reactor, thermodynamic modeling, full scale catalyst performance, BTE engine experiments, analytical measurements, and CFD modeling

Accomplishments

- Developed catalyst operating strategy to continuously produce >15% H_2 without coking
- Successfully implemented catalytic EGR-loop reforming on a multi-cylinder engine, reducing fuel consumption my more than 10% with H_2
- Employed thermodynamic modeling of catalyst and CFD modeling of combustion to provide insight and paths forward on favorable operating conditions

Collaborations

- Ford, Aramco Services Co., Umicore, Ansys, University of Michigan

Future Work

- Address barriers associated with catalytic EGR-loop reforming identified by industry partners
  - Tolerance to sulfur in gasoline, light load engine stability, high load compatibility

Any proposed future work is subject to change based on funding level

Technical Backup Slides

Contacts:

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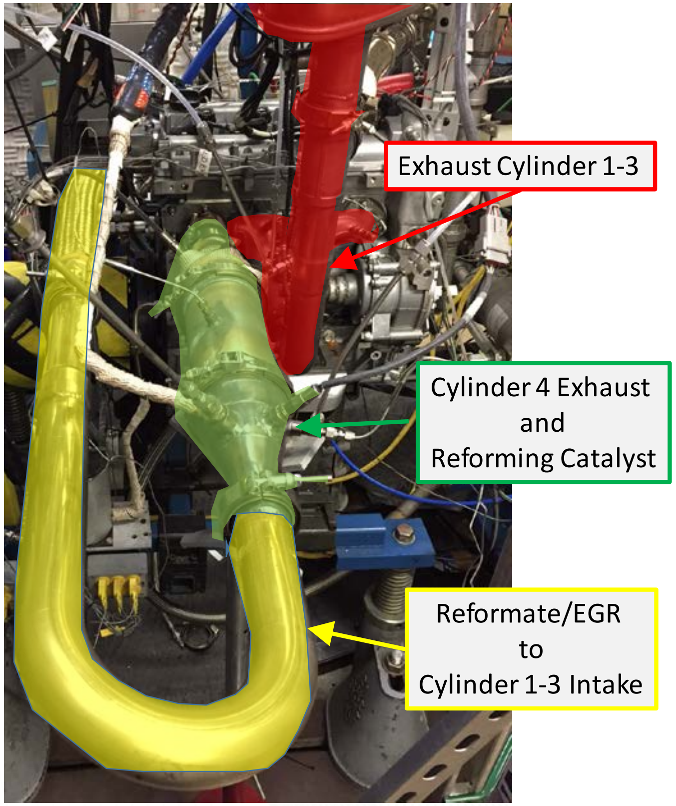
Experimental Details

Backup (1/5)

- Base engine: 2007 GM LNF engine
  - 2.0 L Displacement (bore x stroke: 86 mm x 86 mm)
  - Direct injection (constant rail pressure of 100 bar for this study)
  - Stock pistons and compression ratio (9.2:1)
- Pre-production catalyst from Umicore
  - 2 wt% Rh with an alumina washcoat
  - 1.5 L catalyst volume, cordierite substrate
- Single operating point study: 2000 rpm, 4 bar BMEP
- Engine-out emissions measured with a 5-gas emissions bench
- Additional analyzers used to speciate reformate and exhaust
  - FTIR to speciate hydrocarbons
  - Magnetic sector mass spectrometer used to measure H_2
- Iso-octane and certification gasoline used

Picture of Engine Modified with Reforming Catalyst



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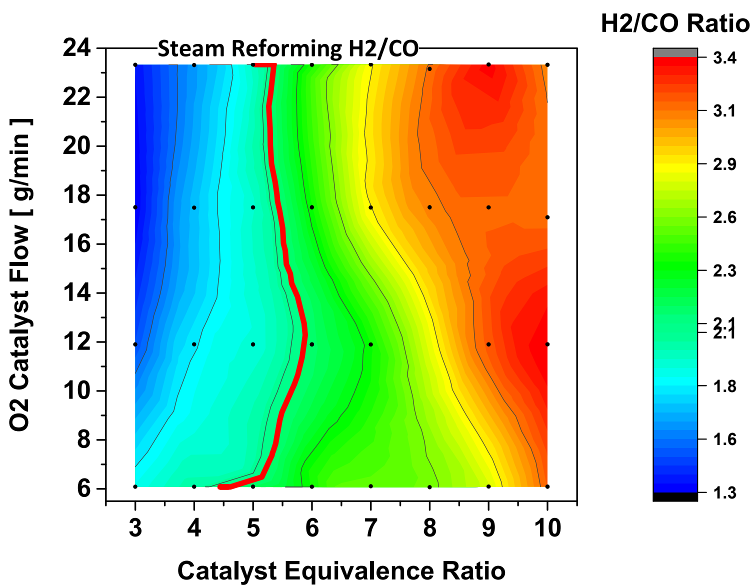
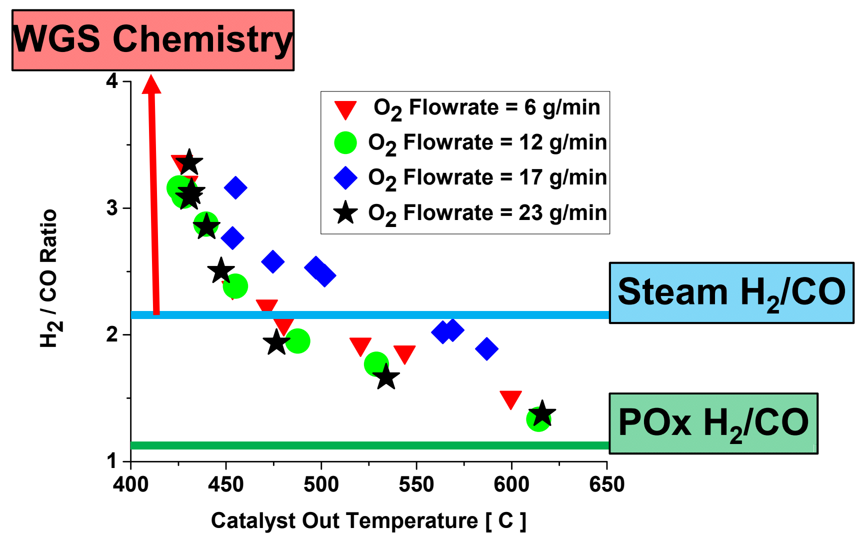
The H_2 to CO Ratio Provides Insight into the Reforming Chemistry

Backup (2/5)

- Partial oxidation reforming of iso-octane produces $H_2/CO = 1.125$ ($C_8H_{18} + 4\ O2 \rightarrow 8\ CO + 9\ H_2$)
  - Experiments show that all operating conditions have a higher H2/CO ratio than POx, but those around $\Phi = 3.0$ approach this limit
- Steam reforming produces $H_2/CO = 2.125$ ($C_8H_{18} + 8\ H_2O \rightarrow 8\ CO + 17\ H_2$)
  - Experimentally, this H_2/CO ratio occurs at $\Phi = 5$ to 6
  - H_2/CO higher than 2.125 can be attributed to water-gas shift (WGS) chemistry
  - Higher H_2/CO ratio is thermodynamically favored at lower temperatures (chemical equilibrium)





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All Data Thus Far Shown with Iso-Octane. What happens with a real fuel?

Backup (3/5)

	Iso-octane	Tier II Lube Cert	Tier II	Tier III
RON	100	97.0	96.8	91.8
MON	100	88.7	88.6	84.2
S	0	8.3	8.3	88
Ethanol [%]	0	0	0	9.8
T10 [deg C]	99	52.2	52.2	54.6
T50 [deg C]	99	104.5	103.3	89.9
T90 [deg C]	99	156.7	155.6	157.8
Sulfur [ppm]	0	7	30	10.2
Carbon [wt %]	84.2	86.5	86.6	82.63
Hydrogen [wt%]	15.8	13.28	13.4	13.66
Oxygen [wt %]	0	<0.01	None Detected	3.71

Fuels Investigated

Reference Fuel Specs

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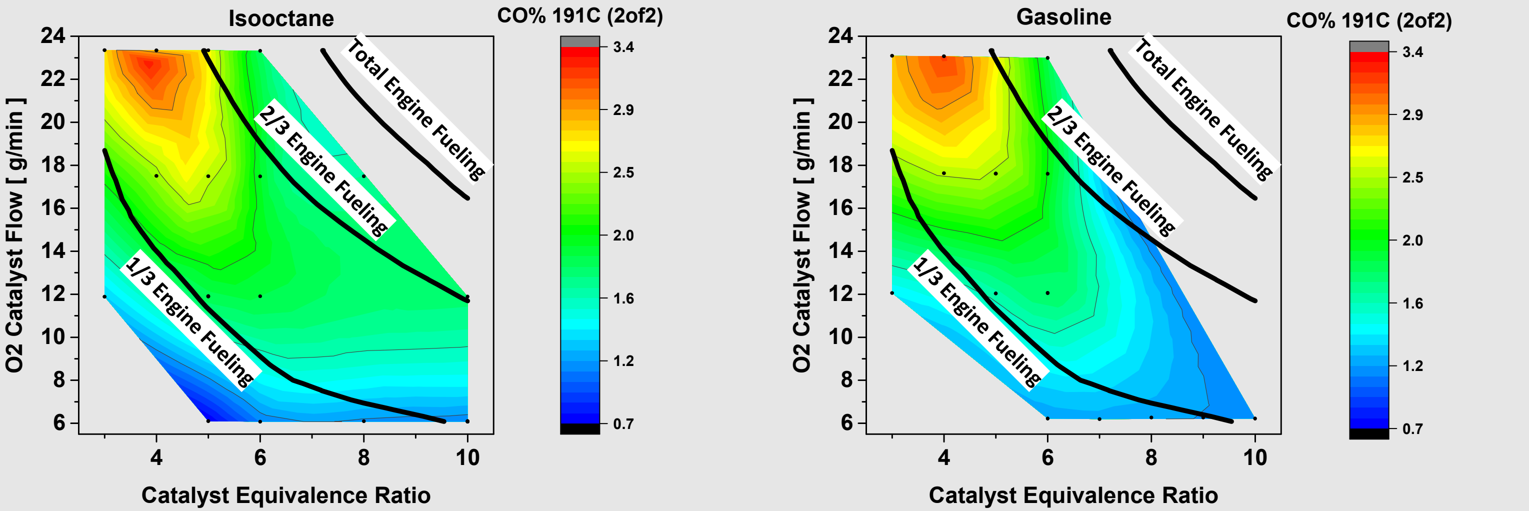
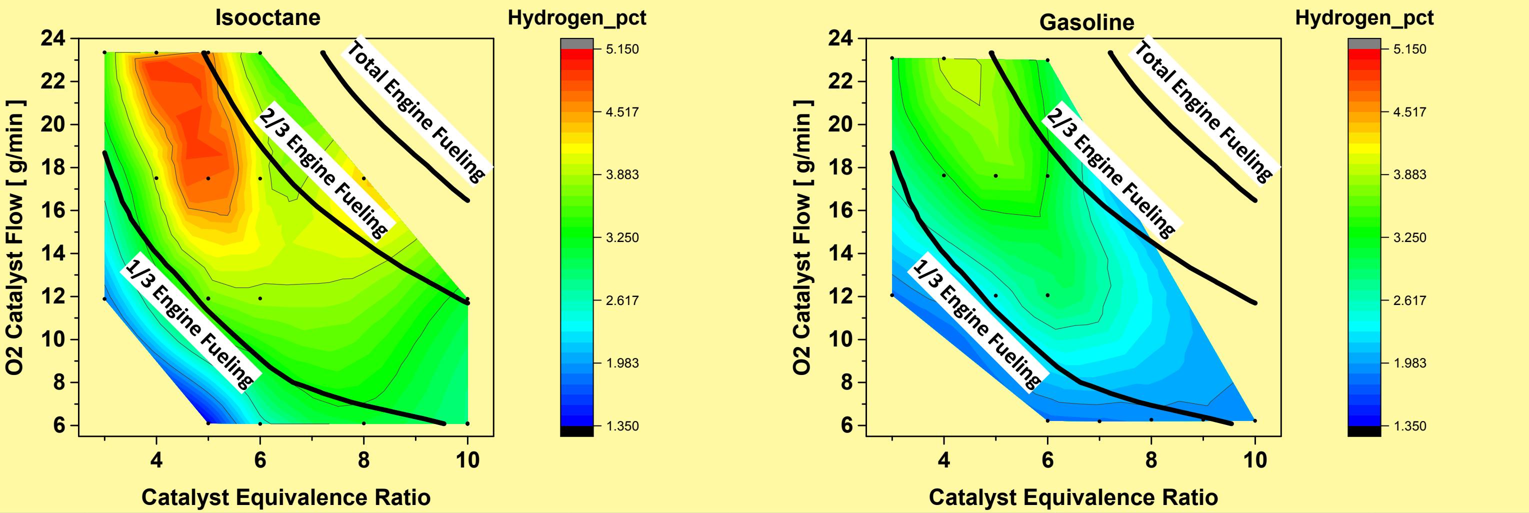
Gasoline CO production is similar, but H_2 is reduced
Reduction Possibly due to Reduce Fuel H/C or Higher Sulfur

Backup (4/5)

CO



H_2



The H_2 to CO Ratio Provides Insight into the Reforming Chemistry

Backup (5/5)

- Partial oxidation reforming of iso-octane produces $H_2/CO = 1.125$ ($C_8H_{18} + 4\ O2 \rightarrow 8\ CO + 9\ H_2$)
  - Experiments show that all operating conditions have a higher H2/CO ratio than POx, but those around $\Phi = 3.0$ approach this limit
- Steam reforming produces $H_2/CO = 2.125$ ($C_8H_{18} + 8\ H_2O \rightarrow 8\ CO + 17\ H_2$)
  - Experimentally, this H_2/CO ratio occurs at $\Phi = 5$ to 6
  - H_2/CO higher than 2.125 can be attributed to water-gas shift (WGS) chemistry
  - Higher H_2/CO ratio is thermodynamically favored at lower temperatures (chemical equilibrium)